ECE 371
Materials and Devices

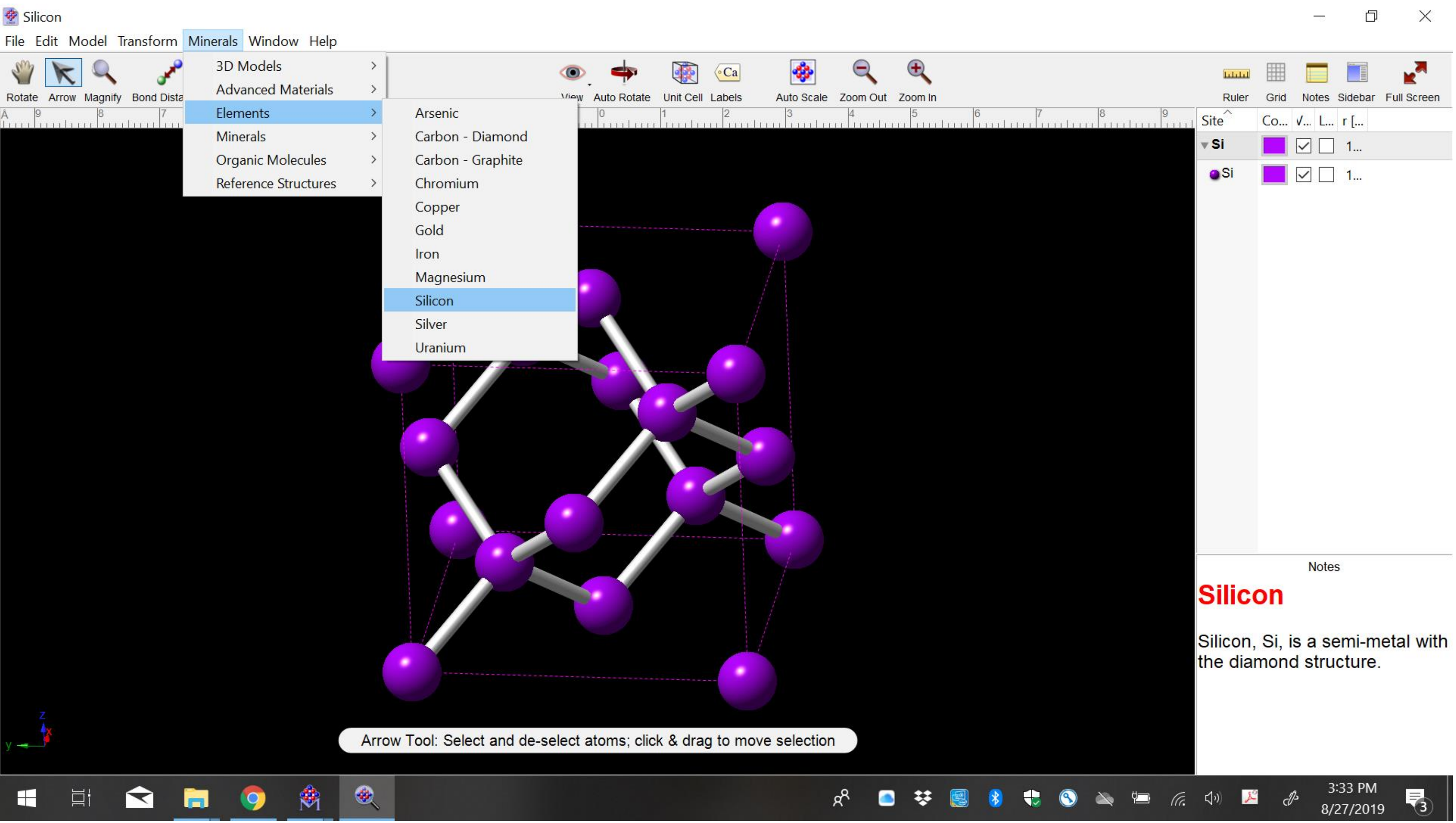
08/29/19 - Lecture 3

Intro to Quantum Mechanics and Schrödinger’s Equation

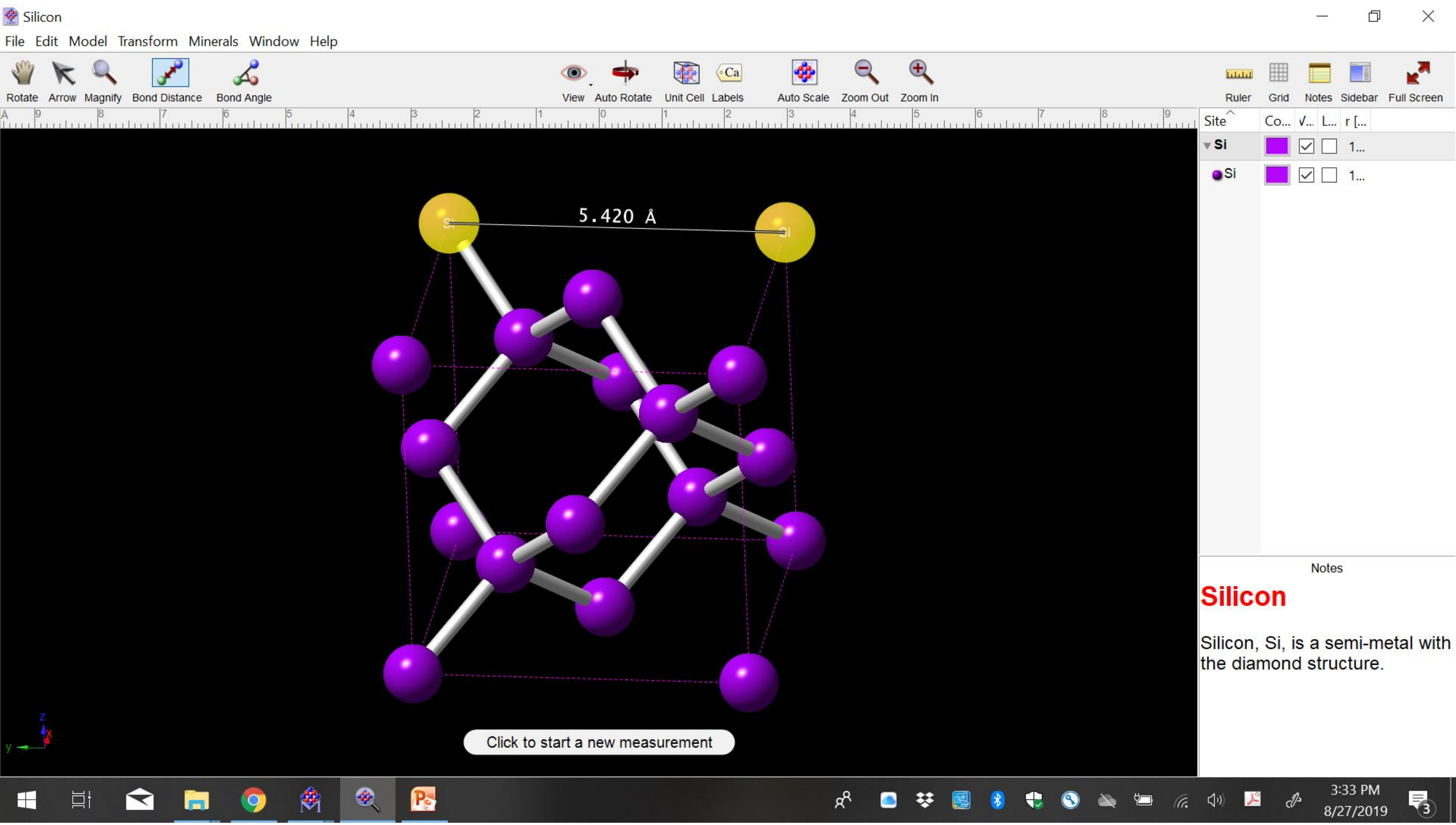
General Information

- Homework #1 assigned and due before class on Tuesday Sept 3rd
- Link to download Crystal Viewer (http://crystalmaker.com/crystalviewer/index.html) added to the website in Articles, Videos, and Additional Notes folder. See next few slides for examples of software capabilities.
- Reading for next time: 2.2.2-2.3.1

View Silicon Structure

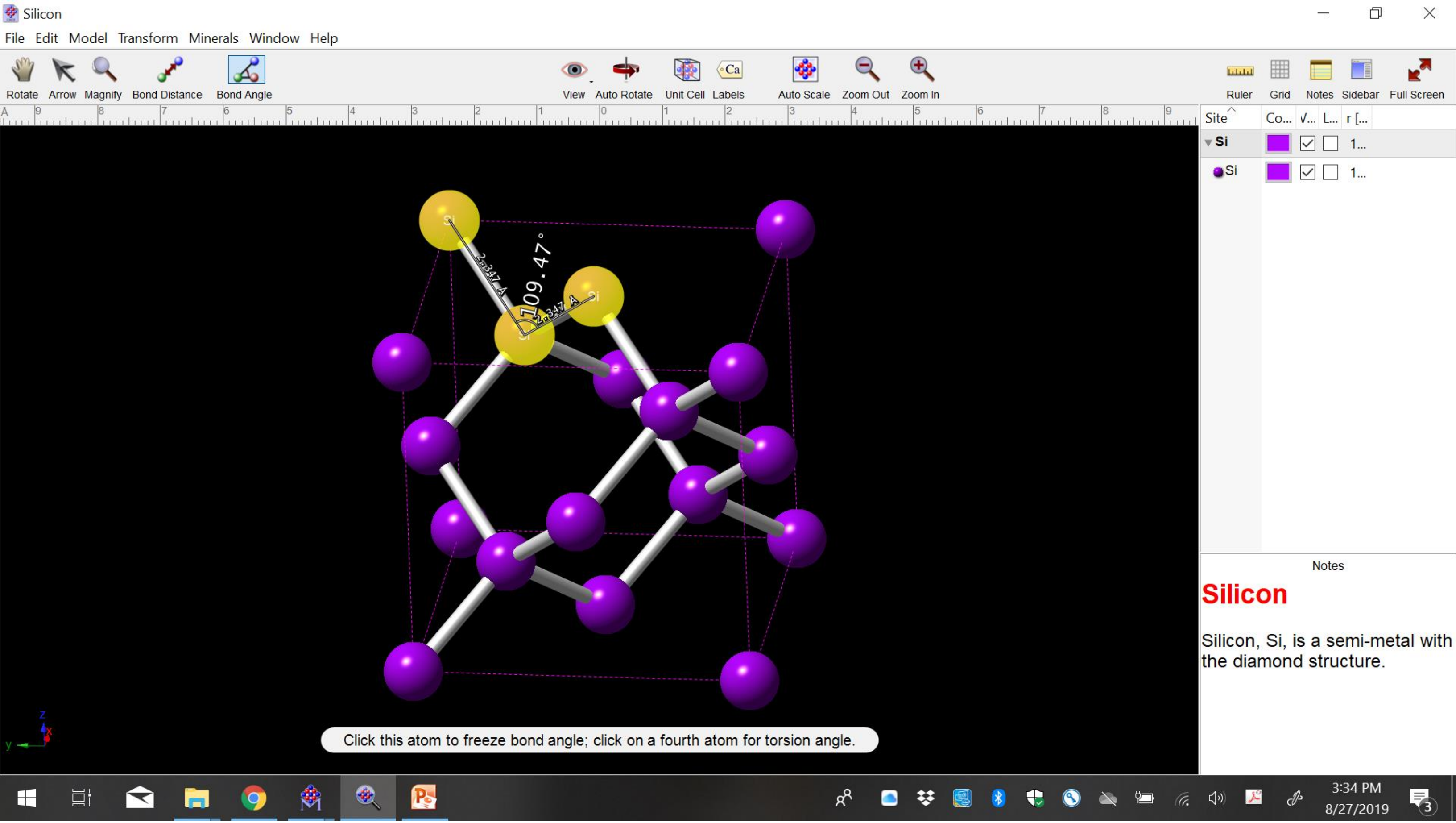


View Bond Distance

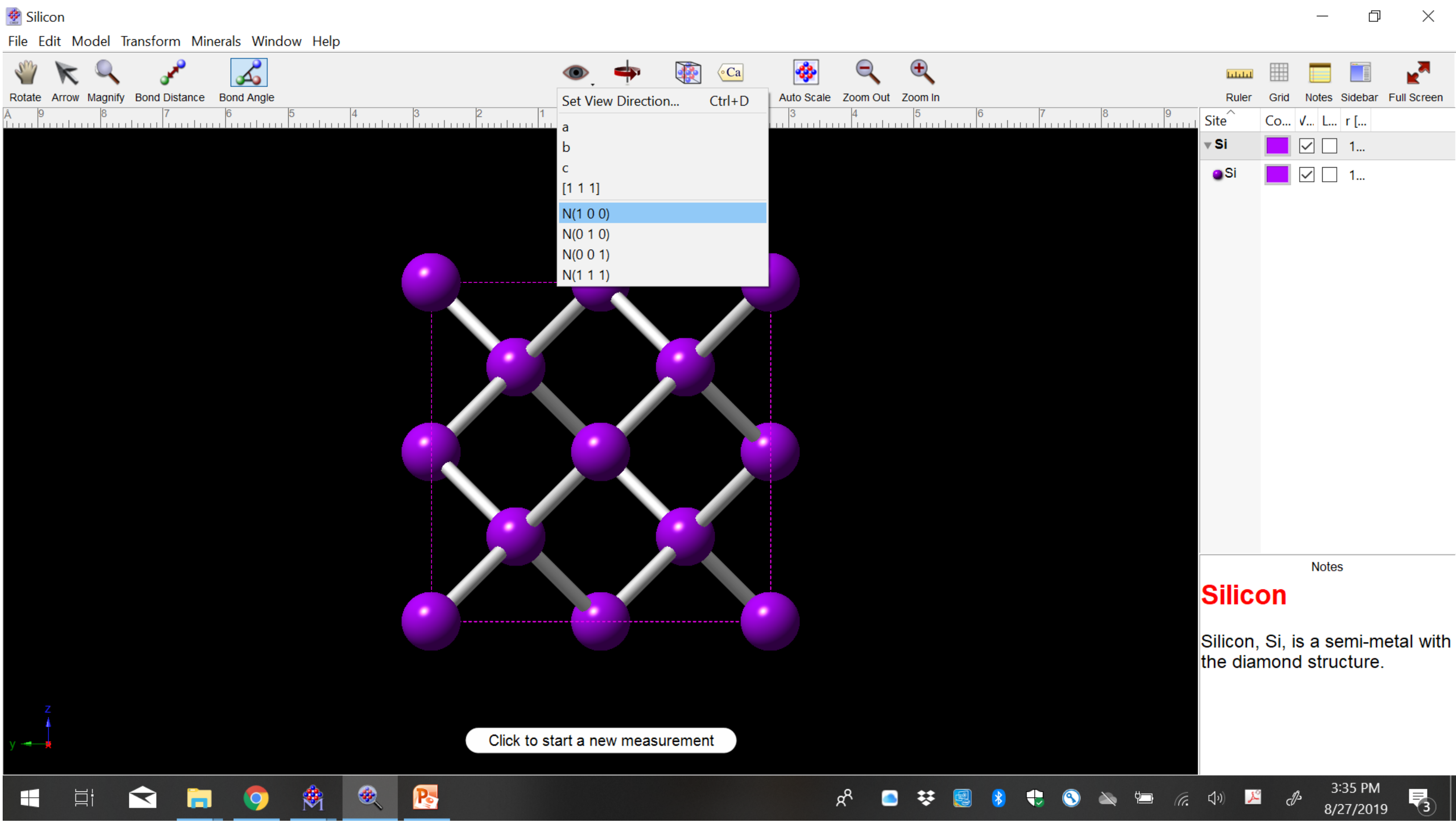


*Useful tool for confirming nearest neighbor atoms

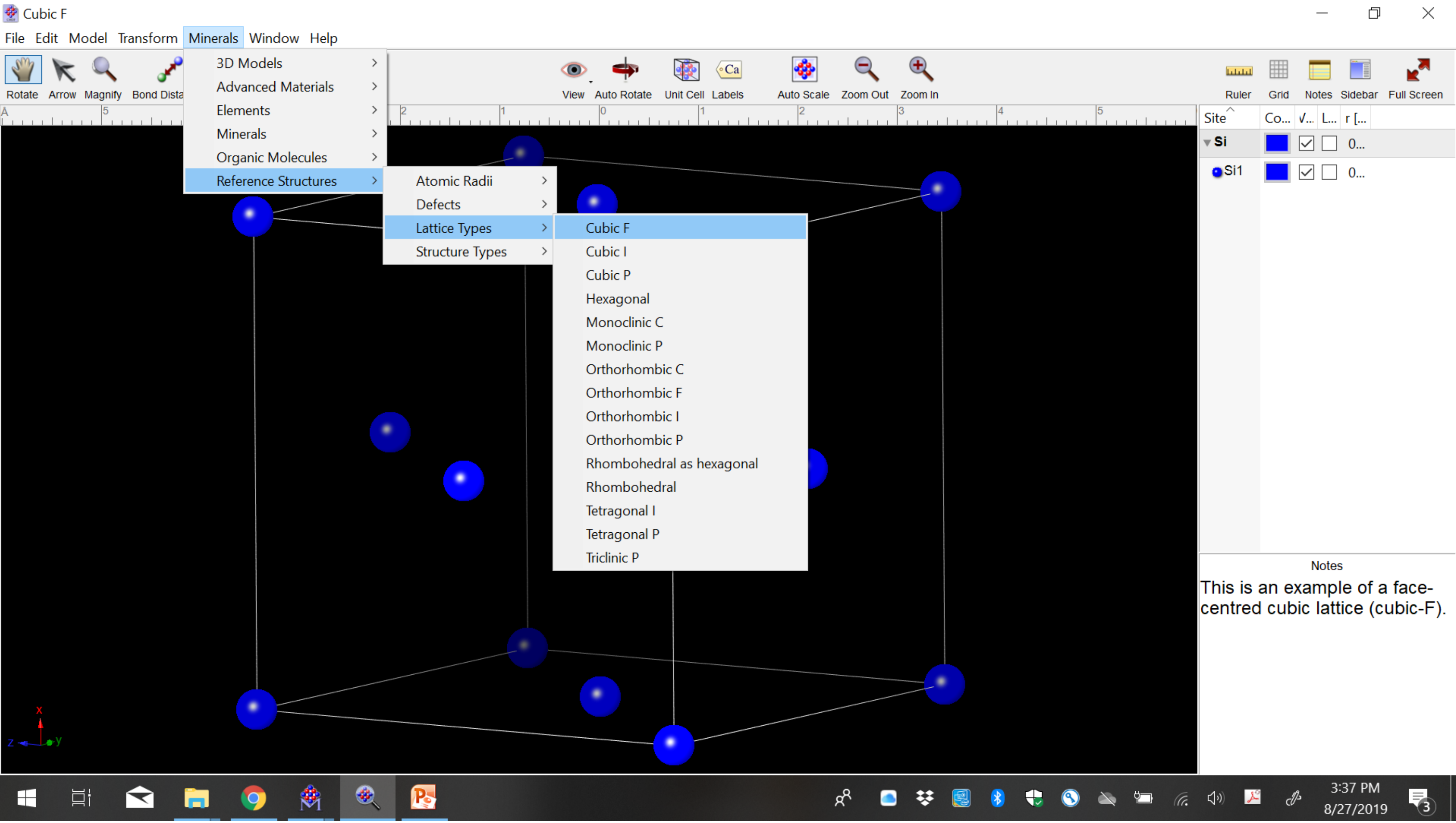
View Bond Angle



Select Direction of View



View SC, BCC, and FCC Structures



Why Do We Need Quantum Mechanics?

- Classical Newtonian mechanics:
  - Works well to explain the behavior of large objects (e.g. – baseball, car)
  - Variables (e.g. – position (x) and momentum (p)) are *continuous (non-discrete)* in nature
  - Time-dependent processes are deterministic in nature
  - Evolution of the whole universe could in theory be predicted!

- However, in the early 1900s, several experimental results were not consistent with classical mechanics

- A new theory called *quantum mechanics* was developed
  - Explains the behavior of small objects (electrons, protons, photons)
  - Physical processes not pre-determined in a mathematically exact sense
  - Variables can be discrete (or "quantized")
  - Schrödinger's Wave Equation is the workhorse of quantum mechanics

- *Semiconductors are governed by the movement of electrons through a crystal lattice and therefore require a quantum mechanical description*

Rayleigh-Jean Law

- At the end of the 19th century, scientists were trying to explain the emission spectrum of a black body radiator

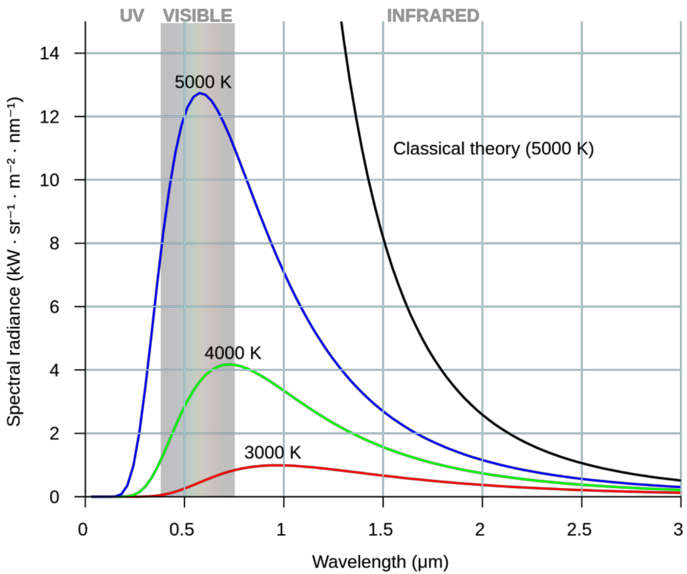


image source: wikipedia

- Classical theory is known as the Rayleigh-Jean Law

$$\boxed{I(\lambda) = \frac{2\pi k T}{\lambda^2}}$$

- Singularity as $\lambda \to 0$ is unphysical and known as the "UV Catastrophe" since the law does not hold for the short wavelength (high frequency) region

- Something was wrong!

The Beginning: Planck's Postulate and Law

- At the end of the 19th century, scientists were trying to explain the emission spectrum of a black body radiator

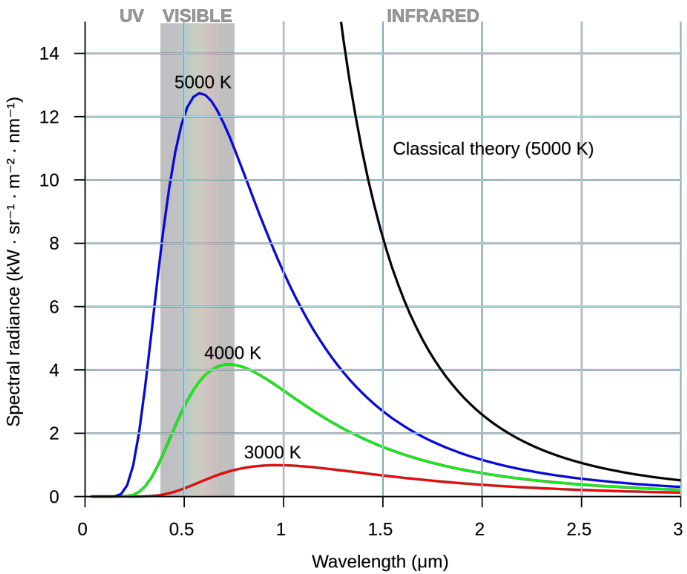


image source: wikipedia

- Planck postulated that the radiation occurred in discrete units of energy (*energy quanta)* in order to explain the radiation spectrum of a perfect black-body radiator
- $E = h\nu, 2h\nu, 3h\nu\ldots$, where h is the Planck constant = 6.63x10^{-34} J s and $\hbar = h/2\pi$
- Using this postulate, Planck derived

$$\boxed{I(\lambda) = \frac{4\pi\hbar c^2}{\lambda^5\left[\exp\left(\frac{2\pi\hbar c}{\lambda k T}\right) - 1\right]}}$$

- Planck's postulate represents the historical origin of quantum mechanics

The Photoelectric Effect

- In 1905, Einstein interpreted an experiment that verified the discrete nature (quantization) and particle-like behavior of light
- Absorption of light by a metal surface and it's relation to the frequency of the light
- Some electrons in the metal receive sufficient energy to be ejected into the vacuum
- The amount of energy required to eject an electron is called the *work function* (Φ)
- The maximum kinetic energy of the ejected electrons depends upon the frequency of the light, showing that $E \propto \nu$
- The number of ejected electrons increases as the light intensity increases but their maximum kinetic energy does not increase, showing that the interaction must be particle like (i.e. – all energy is given to an electron)

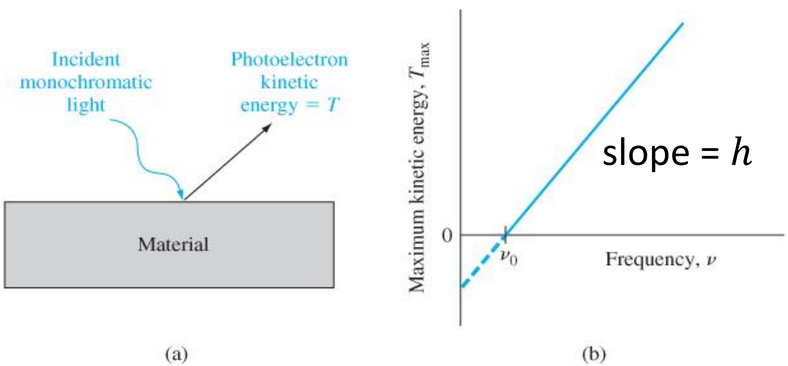


Figure 2.1 | (a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.

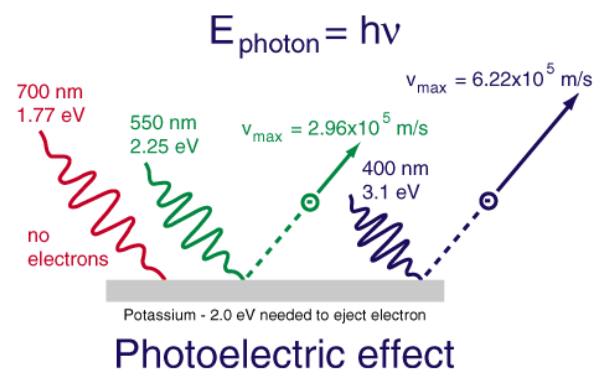


image source: hyperphysics

The Compton Effect

- Provided additional evidence that light can behave as a particle
- Photons behave as "billiard balls" and energy and momentum are conserved
- Photon with energy $h\nu$ transfers some of it's energy to the electron
- Scattered photon has a lower energy ($h\nu'$) than the incident photon

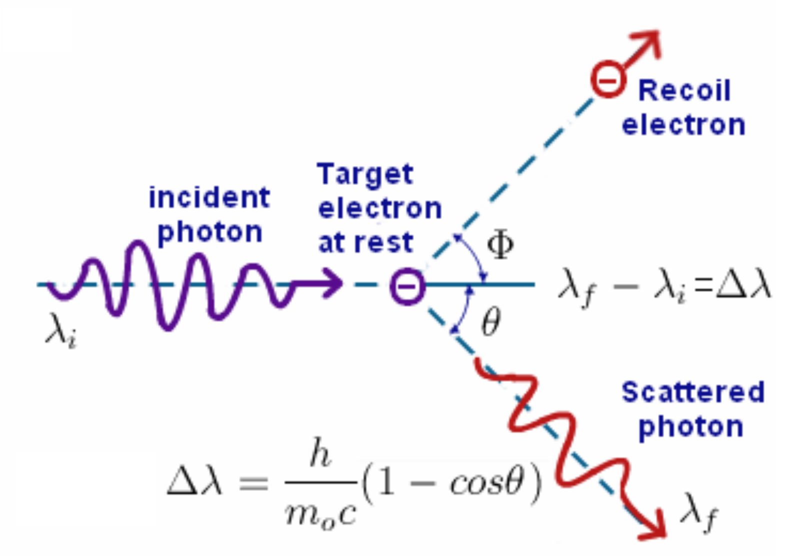


image source: http://physics.tutorvista.com/modern-physics/compton-scattering.html

Wave-Particle Duality

- In 1924, de Broglie postulated the existence of matter waves
- Waves exhibit particle-like behavior so particles should exhibit wave-like behavior

$$\boxed{p = \frac{h}{\lambda}}$$

photon momentum

$$\boxed{\lambda = \frac{h}{p}}$$

de Broglie wavelength

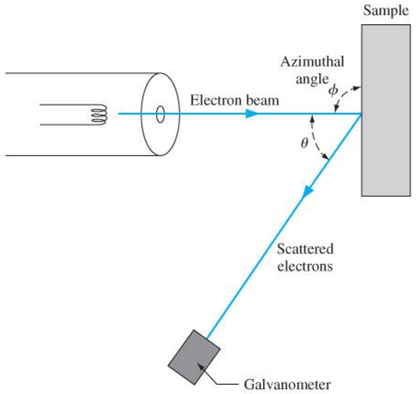


Figure 2.2 | Experimental arrangement of the Davisson–Germer experiment.

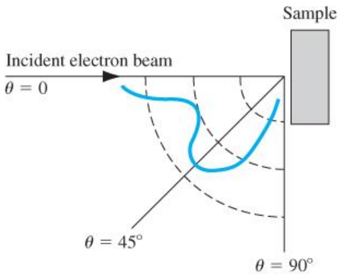


Figure 2.3 | Scattered electron flux as a function of scattering angle for the Davisson–Germer experiment.

*Peaks in the scattered electron flux are interpreted as constructive interference of electron waves scattered by the periodic crystal lattice, similar to light scattered from a diffraction grating

The Electromagnetic Spectrum

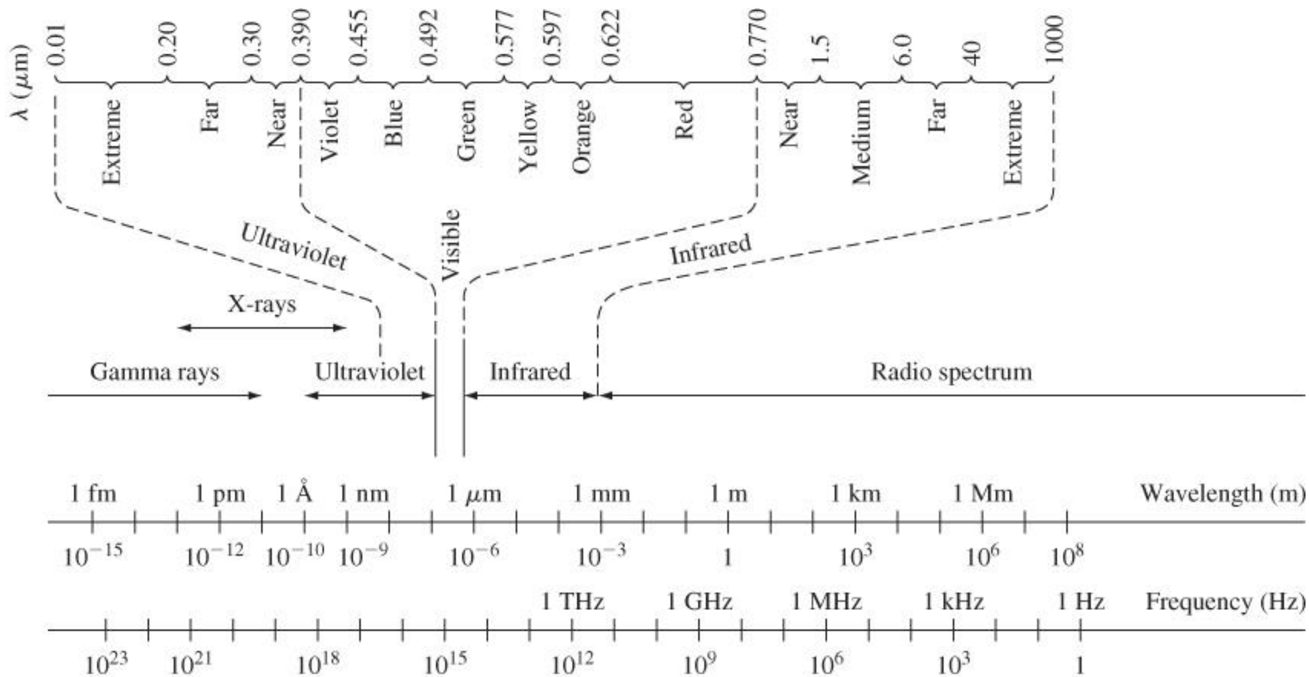


Figure 2.4 | The electromagnetic frequency spectrum.

Questions

- What is the de Broglie wavelength of an electron traveling at 5e6 cm/s?
  - A: 14.5 nm
  - B: 1.45 Å
  - C: 72.7 Å
  - D: 72.7 nm

- What is the de Broglie wavelength of a cyclist with mass 70 kg going 9 m/s?
  - A: 85.3 nm
  - B: 1023 m
  - C: 1.1e-36 m
  - D: 2.7e-15 m

The Uncertainty Principle

- Quantum mechanical systems do not allow for predictions of their future state with arbitrary accuracy
- The *Heisenberg Uncertainty Principle* allows us to quantify the uncertainty associated with quantum mechanical particles

Formulations of the Uncertainty Principle

1. It is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle

$$\boxed{\Delta p\,\Delta x \;\geq\; \hbar}$$

1. It is impossible to describe with absolute accuracy the energy of a particle and the instance of time the particle has this energy

$$\boxed{\Delta E\,\Delta t \;\geq\; \hbar}$$

We can only make predictions for subatomic particles in terms of a *probability distribution*

Wave Function

- The temporal and spatial evolution of a particle (e.g., electron) with one degree of freedom is given by $\psi(x,t)$
- $\psi(x,t)$ can be complex
- $\psi(x,t) \cdot \psi^*(x,t)$ is related to the probability of finding the particle within the interval $x + dx$
- The shape of the wave function is influenced by the potential energy landscape

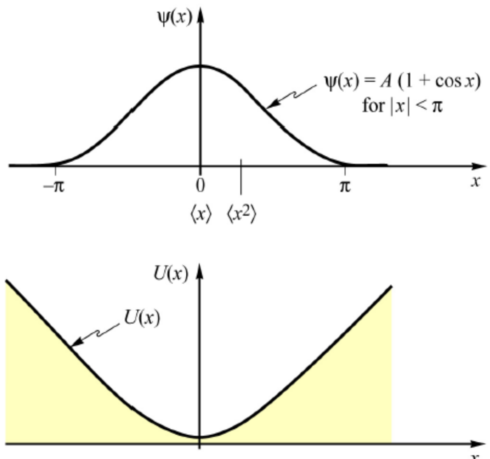


Fig. 2.1. Example for a one-dimensional wave function ψ(x). Also shown is a corresponding potential function, U(x). This potential function provides a driving force towards x = 0, that is towards minimum energy.

Schubert, “Physical Foundations of Solid State Devices”

Schrödinger's Wave Equation

- The Schrödinger equation (SE) describes the spatial and temporal evolution of the wave function for a given potential energy landscape and set of boundary conditions

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = j\hbar\frac{\partial\psi(x,t)}{\partial t}}$$

related to kinetic energy

related to potential energy

related to total energy

- $V(x)$ is the potential energy, m is the mass of the particle, and $j = \sqrt{-1}$
- SE is a basic postulate of quantum mechanics but can be derived
- SE can be used to describe the behavior of electrons in a crystal

Time-Dependent and Time-Independent Parts of SE

- The separation of variables technique can be used to deconstruct the SE into time-dependent and time-independent parts
- We assume that the wave function can be represented as the product of a time-independent function and a time-dependent function (i.e., $\psi(x,t) = \psi(x)\phi(t)$)

Time-dependent solution can be obtained quickly:

$$\boxed{\phi(t) = e^{-j\left(\frac{E}{\hbar}\right)t} = e^{-j\omega t}}$$

Sinusoidal variation with time
E is the total energy of the particle

Time-independent part of the equation:

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi(x) = 0}$$

Nature of the solution for $\psi(x)$ depends upon the potential V(x) and the boundary conditions

*see in-class derivation